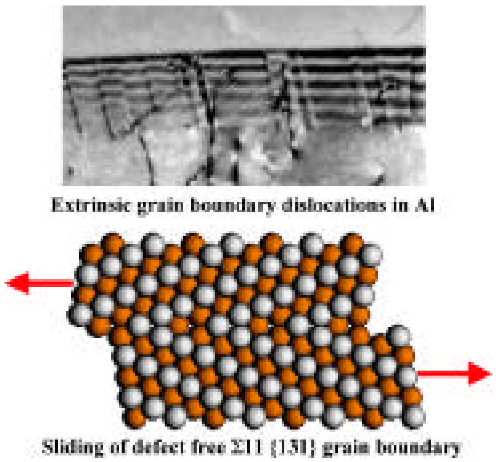
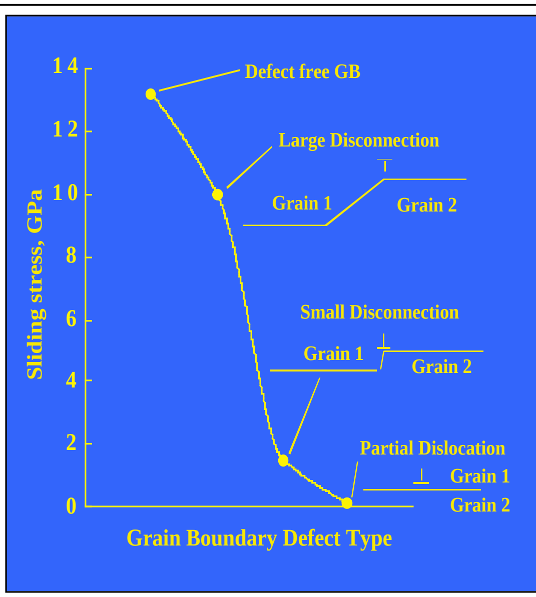
VI.E Grain Sliding for Superplastic Deformation of Aluminum

Introduction: The fuel efficiency of the automobile increases as the weight of the automobile decreases. This simple relationship is driving a large nationwide effort to develop new low cost, robust, lightweight alloys for multiple uses on the car. However, until the cost of processing can become competitive with sheet steels, the cost to produce automobiles using significant amounts of aluminum is prohibitive. To reduce the cost of processing, it is necessary to rapidly form the alloy. Rapid forming is possible with aluminum because, under the right conditions, it "superplastically" deforms. Superplastic deformation involves low-stress sliding along grain boundaries, a complex process of which material scientists have limited knowledge. Experimentalists are not able to directly measure the force or stress required to slide the aluminum along a grain boundary. Therefore, it is necessary to rely on realistic simulations to provide a measure of this invaluable material property.



Computer model of grain boundary sliding

Calculational Notes: The calculations involve molecular dynamics relaxations using the embedded atom potential for Al. It simulates 2,000 movable atoms with flexible borders for 2,000 relaxation steps to minimize the energy. The calculation is done at 0°K with up to 20,000 atoms for a chain-of-states method to analyze the energy barrier to grain sliding. The simulation ran on a HP C-160 workstation.



Computed sliding stress for various boundary defects

Results: Simulating the atoms in a chunk of aluminum provides opportunities for gaining understanding of the mechanisms underlying sliding processes. The figure to the left shows the calculated stress that is necessary to slide a grain boundary in aluminum. The simulations also analyze and provide information about the energy barriers to the grain sliding.

Significance: These simulations are providing essential input needed for the rational design of improved aluminum alloys. The ability to analyze the sliding resistance of a single grain boundary with and without various defects is an example of a new way of doing science. With SSI resources, it will become possible to provide increasing guidance in the development of new, more formable alloys instead of relying on trial and error.